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DEPARTMENT OF MATHEMATICAL SCIENCES
COLLEGE OF SCIENCES
OLD DOMINION UNIVERSITY
NORFOLK, VIRGINIA 23529

THEORETICAL STUDIES OF SOLAR LASERS AND CONVERTERS

By

John H. Heinbockel, Principal Investigator

Progress Report
For the period May 15 to December 31, 1988

Prepared for the
National Aeronautics and Space Administration
Langley Research Center
Hampton, Virginia 23665-5225

Under
Research Grant NAG-1-757
Dr. R.C. Costen, Technical Monitor
SDD-High Energy Sci Branch

(NASA-CR-184589) THEORETICAL STUDIES OF SOLAR LASERS AND CONVERTERS Progress Report, 15 May - 31 Dec. 1988 (Old Dominion Univ.) 42 p CSCL 20E

N89-17214

Unclas
G3/36 0178597

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Submitted by the
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P.O. Box 6369
Norfolk, Virginia 23508-0369

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Theoretical Studies of Solar Lasers and Converters

A second computer program has been developed for the simulation of an $n - C_3F_7I$ iodine laser. This computer program is given in the Appendix A and typical output from the computer program is illustrated in the Appendix B.

Chemical Kinetics

The computer program simulates the chemical kinetics occurring during the operation of an $n - C_3F_7I$ iodine laser. Letting R denote the radical $n - C_3F_7$, these reactions are summarized as follows:

Photodissociation of RI and I_2:

$$RI + h\nu_1 \xrightarrow[\xi_1]{0.27\mu m} R + I^*$$

$$I_2 + h\nu_2 \xrightarrow[\xi_2]{0.5\mu m} I + I^*$$

Laser action (stimulated emission)

$$I^* + h\nu_3 \xrightarrow{1.32\mu m} I + 2h\nu_3$$

Quenching of I^* (reaction rates have units $[cm^3/sec]$)

$$I^* + RI \xrightarrow{Q_1} I + RI$$

$$I^* + I_2 \xrightarrow{Q_2} I + I_2$$

$$I^* + R \xrightarrow{Q_3} I + R$$

$$I^* + R_2 \xrightarrow{Q_4} I + R_2$$

$$I^* + I \xrightarrow{Q_5} I + I$$

RI generation and two body recombinations (reaction rates have units $[cm^3/sec]$)

$$R + I^* \xrightarrow{k_1} RI$$

$$R + I \xrightarrow{k_2} RI$$

$$R + R \xrightarrow{k_3} R_2$$

$$R + RI \xrightarrow{k_4} R_2 + I$$

$$R + I_2 \xrightarrow{k_5} RI + I$$

$$R + RI \xrightarrow{k_6} R_2 + I^*$$

$$RI + I^* \xrightarrow{k_7} I_2 + R$$

$$I + RI \xrightarrow{k_8} I_2 + R$$

I_2 formation (reaction rates have units $[cm^6/sec]$)

$$I^* + I + RI \xrightarrow{c_1} I_2 + RI$$
$$I + I + RI \xrightarrow{c_2} I_2 + RI$$
$$I^* + I + I_2 \xrightarrow{c_3} I_2 + I_2$$
$$I + I + I_2 \xrightarrow{c_4} I_2 + I_2$$
$$I + I + R_2 \xrightarrow{c_5} I_2 + R_2$$
$$I + I^* + R_2 \xrightarrow{c_6} I_2 + R_2$$

Wall reactions (reaction rates have units $[cm^3/sec]$)

$$I + I + wall \xrightarrow{v_1} I_2 + wall$$
$$R_2 + I + wall \xrightarrow{v_2} R + RI + wall$$

Reaction rate coefficients

The reaction rate coefficients are assumed to satisfy the following inequalities:

$$.476(10^{-16}) \leq Q_1 \leq 8.4(10^{-16})$$
$$.730(10^{-11}) \leq Q_2 \leq 4.94(10^{-11})$$
$$1.23(10^{-18}) \leq Q_3 \leq 11.1(10^{-18})$$
$$1.57(10^{-16}) \leq Q_4 \leq 14.1(10^{-16})$$
$$.530(10^{-14}) \leq Q_5 \leq 4.8(10^{-14})$$

$$0.9(10^{-13}) \leq k_1 \leq 34.7(10^{-13})$$
$$.657(10^{-11}) \leq k_2 \leq 8.05(10^{-11})$$
$$.65(10^{-12}) \leq k_3 \leq 10.4(10^{-12})$$
$$1.0(10^{-16}) \leq k_4 \leq 9.0(10^{-16})$$
$$0.33(10^{-11}) \leq k_5 \leq 3.0(10^{-11})$$
$$1.0(10^{-17}) \leq k_6 \leq 10.24(10^{-17})$$
$$1.5(10^{-19}) \leq k_7 \leq 4.5(10^{-19})$$
$$0.533(10^{-23}) \leq k_8 \leq 4.8(10^{-23})$$

$$1.0(10^{-33}) \leq c_1 \leq 10.2(10^{-33})$$
$$1.6(10^{-32}) \leq c_2 \leq 45.0(10^{-32})$$
$$4.44(10^{-32}) \leq c_3 \leq 14.4(10^{-32})$$
$$2.92(10^{-30}) \leq c_4 \leq 4.94(10^{-30})$$
$$3.6(10^{-31}) \leq c_5 \leq 6.0(10^{-31})$$
$$1.35(10^{-32}) \leq c_6 \leq 2.25(10^{-32})$$

$$0.33(10^{-12}) \leq v_1 \leq 3.0(10^{-12})$$
$$0.33(10^{-11}) \leq v_2 \leq 3.0(10^{-11})$$

Other coefficients

In the computer program we let: Q_y denote the quantum yield; ξ_1, ξ_2 denote the photodissociation rates which are dependent upon the solar simulator concentration c_0; σ denotes the stimulated emission cross section and ρ denotes the photon density in the optical cavity. We use the approximations

$$\xi_1 = 3.04(10^{-3})c_0, \qquad \xi_2 = 3.38(10^{-2})c_0$$

The pumping is assumed to occur over an interval $0 \le z \le z_L$ where L is the length of the tube. Various assumptions can be incorporated concerning the pumping intensity. Currently, the program assumes that the maximun pumping intensity occurs at $z_{0L} = \frac{1}{2}z_L$.

Differential equations for chemical kinetics

Using the notation $[A]$ to denote the concentration of species A in units of cm^{-3}, the differential equations defining the chemical kinetics for the iodine lase can be expressed by the following set of coupled nonlinear differential equations involving the concentrations $[RI]$, $[R]$, $[R_2]$, $[I_2]$, $[I^*]$, $[I]$.

$$\begin{aligned}
\frac{d[RI]}{dt} &= k_1[R][I^*] + k_2[R][I] + k_5[R][I_2] - k_7[I^*][RI] - k_4[R][RI] \\
&\quad - k_6[R][RI] - \xi_1[RI] + v_2[R_2][I] - k_8[I][RI] \\
\frac{d[R]}{dt} &= \xi_1[RI] - k_1[R][I^*] - k_2[R][I] - 2k_3[R]^2 - k_4[RI][R] \\
&\quad - k_6[RI][R] - k_5[R][I_2] + v_2[R_2][I] + k_7[RI][I^*] + k_8[I][RI] \\
\frac{d[R_2]}{dt} &= K_3[R]^2 + k_6[RI][R] + k_4[RI][R] - v_2[R_2][I] \\
\frac{d[I_2]}{dt} &= c_1[RI][I^*][I] + c_2[RI][I]^2 + c_3[I_2][I^*][I] + c_4[I_2][I]^2 \\
&\quad - \xi_2[I_2] + k_7[RI][I^*] - k_5[R][I_2] + v_1[I]^2 \\
&\quad c_5[I]^2[R_2] + k_8[RI][I] + c_6[I][I^*][R_2] \\
\frac{d[I^*]}{dt} &= Q_y\xi_1[RI] + \xi_2[I_2] - k_1[R][I^*] - Q_2[I_2][I^*] \\
&\quad - c\sigma\rho([I^*] - \frac{1}{2}[I]) + k_6[R][RI] - Q_3[R][I^*] - Q_4[R_2][I^*] \\
&\quad - Q_5[I^*][I] - k_7[RI][I^*] - C_6[R_2][I^*][I] - C_1[RI][I^*][I] \\
&\quad - C_3[I_2][I^*][I] - Q_1[RI][I^*] \\
\frac{d[I]}{dt} &= \xi_2[I_2] + Q_1[RI][I^*] + Q_2[I_2][I^*] - 2c_5[I]^2[R_2] - k_8[I][RI] \\
&\quad + c\sigma\rho([I^*] - \frac{1}{2}[I]) - c_1[RI][I^*][I] - 2c_2[RI][I]^2 - c_3[I_2][I^*][I] \\
&\quad + 2c_4[I_2][I]^2 - k_2[R][I] + k_4[RI][R] + Q_3[I^*][R] + Q_4[I^*][R_2] \\
&\quad + Q_5[I^*][I] + k_5[R][I_2] - v_2[R_2][I] - 2v_1[I]^2 - c_6[R_2][I^*][I]
\end{aligned}$$

In the above differential equations we use the material derivative

$$\frac{d[A]}{dt} = \frac{\partial[A]}{\partial t} + \frac{\partial[A]}{\partial z}\frac{dz}{dt} = \frac{\partial[A]}{\partial t} + \frac{\partial[A]}{\partial z}\omega$$

where $\frac{dz}{dt} = \omega$ is the flow rate in the axial direction.

The above system of nonlinear differential equations conserves the masses of the species involved in the reactions and for steady state operation at any point z we have the immediate integrals

$$[RI] + [R] + 2[R_2] = constant$$
$$[RI] + 2[I_2] + [I^*] + [I] = constant$$

Photon density

For the light flux density of lasing photon ρ we let $\rho = \rho_+ + \rho_-$ where $\rho_+ = \rho_+(z,t)$ denotes the photon density propagating in the positive z direction and $\rho_- = \rho_-(z,t)$ denotes the photon density propagating in the negative z direction. The differential equations for these photon densities are given by

$$\frac{1}{c}\frac{\partial \rho_+}{\partial t} + \frac{\partial \rho_+}{\partial z} = \sigma[I^*]\,\rho_+\,([I^*] - \frac{1}{2}[I])$$
$$\frac{1}{c}\frac{\partial \rho_-}{\partial t} - \frac{\partial \rho_-}{\partial z} = \sigma\rho_-([I^*] - \frac{1}{2}[I])$$

where c is the speed of light in the optical medium. In the above equations $\sigma[I^*]\rho_+$ is the amplification factor resulting from population of the upper lasing level of the active medium and $-\frac{1}{2}\sigma[I]\rho_+$ is the decrease in photon density due to population of the lower lasing level.

Compressible flow

The effects of fluid density variation as a function of distance z along the tube is considered. Also the pressure and temperature of the flow medium are calculated as a function of distance z and incorporated into the computer model by including the following equations:

(i) An equation of state:

For P the pressure in the gas, T the absolute temperature, and η the gas density, we assume an equation of state for a perfect gas

$$P = \eta RT$$

where R is the universal gas constant.

(ii) Continuity equation (conservation of mass):

The continuity equation is expressed

$$\frac{\partial \eta}{\partial t} + div\,(\eta\vec{V}) = 0$$

where η is the gas density and $\vec{V}$ is the gas velocity. For steady state conditions and $\vec{V} = \omega\hat{k}$ the flow in the axial direction, the continuity equation reduces to

$$\frac{\partial}{\partial z}(\eta\omega) = 0$$

which implies that

$$\eta\omega = constant.$$

(iii) Momentum equation

The momentum equation for a control volume having a mass $\eta d\tau$ where $d\tau$ is an element of volume, is given by

$$\vec{M} = \iiint \vec{V}\eta d\tau.$$

Using Newton's second law we have

$$\vec{F} = \frac{D\vec{M}}{Dt} = \frac{D}{Dt}\iiint \vec{V}\eta d\tau$$

where $\frac{D}{Dt}$ is the material derivative. We have that

$$\frac{D\vec{M}}{Dt} = \iint \vec{V}(\eta\vec{V}\cdot d\vec{\sigma}) + \frac{\partial}{\partial t}\iiint \vec{V}\eta d\tau$$

where the surface integral term above represents the efflux of momentum through the control volume and the volume integral term represents the change in momentum inside the control volume. Changing the surface integral to a volume integral by using the Gauss divergence theorem

$$\iint \vec{V}(\eta\vec{V}\cdot d\vec{\sigma}) = \iiint \left[\nabla\cdot\eta\vec{V}\vec{V}\right]\,d\tau$$

and letting $\vec{F} = \iiint \vec{f}\, d\tau$ where $\vec{f}$ is the average force per unit volume, we obtain

$$\vec{F} = \iiint \vec{f}\, d\tau = \iiint \left[\frac{\partial}{\partial t}(\eta\omega)\hat{k} + \frac{\partial}{\partial z}(\eta\omega^2)\hat{k}\right] d\tau$$

where $\vec{V}\vec{V} = \omega^2\hat{k}\hat{k}$ is a dyadic and $\vec{f} = -\nabla P$ is the average force per unit volume which is due to the fluid pressure P. This equation implies that

$$-\frac{\partial P}{\partial z} = \frac{\partial}{\partial t}(\eta\omega) + \frac{\partial}{\partial z}(\eta\omega^2).$$

Using the result $\eta\omega = c_1 =$ a constant, the steady state form of the above gives us

$$-\frac{\partial P}{\partial z} = c_1\frac{\partial \omega}{\partial z}$$

and an integration gives

$$P + c_1\omega = c_2$$

where c_2 is a constant of integration.

Energy equation

In terms of the specific enthalpy h per unit mass, the energy equation for the gas flow can be expressed

$$\eta\frac{Dh}{Dt} = \frac{DP}{Dt} + \kappa\nabla^2 T + q$$

where P is the pressure, T is the absolute temperature, κ is the thermal conductivity, and $q = q(z)$ is the raditation heat flux. In one dimension, the energy equation can be expressed

$$\eta\frac{\partial h}{\partial t} + \eta\omega\frac{\partial h}{\partial z} = \frac{\partial P}{\partial t} + \omega\frac{\partial P}{\partial z} + \kappa\frac{d^2T}{dz^2} + q.$$

For C_p the specific heat at constant temperature and C_v the specific heat at constant volume, we can write $h = C_pT$ and $C_p - C_v = R$. This gives us the steady state equation

$$\eta\omega[C_v(T) + R]\frac{dT}{dz} = \omega\frac{dP}{dz} + \kappa\frac{d^2T}{dz^2} + q$$

where we have neglected the effects of viscosity. If we also neglect the effects of the thermal conductivity the above equation reduces to

$$c_1[C_v(T) + R]dT + \omega c_1 d\omega + q dz = 0$$

Using the empirical model

$$C_v(T) = \alpha_v \exp(\beta_v(T - 300)), \qquad 298.15 \le T \le 500$$

where $\alpha_v = 147.23$ and $\beta_v = 0.0012$ are constants, the above equation can be integrated to obtain

$$c_1\frac{\alpha_v}{\beta_v}\exp(\beta_v(T - 300)) + c_1R(T - 300) + \frac{1}{2}c_1\omega^2 - Q = c_4$$

where

$$Q = \int q(z)\, dz$$

and c_4 is a constant of integration.

Computer program

The above equations can be found in the computer program listed in the Appendix A. This program can be described as follows:

Main program

This assigns values to all constants and parameters and then guesses at an initial photon density. The equations are then integrated from 0 to L and the boundary conditions (discussed in an earlier report) are checked to see if they are satisfied. If they are not satisfied then an iterative scheme is employed to find the initial photon density which satisfies the boundary conditions. When the correct initial photon density is used the results of the computations are printed out.

Subroutine GRAPHS

Produces graphical output for each of the species concentration as a function of distance z in the axial direction.

Subroutine PFLOW

This subroutine calculates certain parameters needed in subroutine FLOW. These parameters are stored in common BLK10.

Subroutine FLOW

This subroutine calculates the temperature T, pressure P, flow rate W, density η, Pressure in torr, as a function of axial distance z.

Subroutine ARREN

This subroutine calculates how some of the rate coefficients change with temperature where we have assumed various arrenhius expressions for the different rate coefficients. Other rate coefficients are held constant.

Subroutine CHSI1

This subroutine calculates ξ_1 as a function of z.

Subroutine CHSI2

This subroutine calculates ξ_2 as a function of z.

Subroutine COEFFS

This subroutine calculates the various constants and rate coefficients needed for execution of the program.

Subroutine VELOC

This subroutine calculates the velocity ω as a function of tube radius. Various assumed flow patterns can be assumed. Current version assumes a parabolic flow profile with the velocity of the gas going to zero at the tube walls.

Subroutine FUN

This subroutine calculates the functions occuring on the right hand side of the differential equations to be solved.

Subroutine SIGMA

This subroutine calculates the absorption cross section σ.

Subroutine INTEG

This subroutine integrates the differential equations from 0 to z using a 7th order Runge-Kutta-Fehlberg variable step size integration routine.

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A P P E N D I X   A

```
      PROGRAM CFLM1(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE8)
C     MAIN PROGRAM
C     COMPRESSIBLE FLOW LASER MODEL WHICH INCLUDES
C          EQUATION OF STATE
C          CONTINUITY EQUATION
C          MOMENTUM EQUATION
C          ENERGY EQUATION
C
C        USED IN PREDICTION MODE---GIVEN CONDITIONS AT Z=0.
C
C
C     THIS VERSION CONTAINS AN AUTOMATICALLY CHOSEN VARIABLE STEP
C     SIZE.  IT ALSO CONTAINS WALL EFFECT REACTIONS.(NOT USED THOUGH)
C
C      EFFECTS OF TEMPERATURE, FLOWRATE,DENSITY AND PRESSURE VARIATIONS
C      ARE CONSIDERED IN SUBROUTINES ARREN, PFLOW AND FLOW
      COMMON/BLK2/K1,K2,K3,K4,K5,K6,K7,K8,C1,C2,C3,C4,C5
      COMMON/BLK27/Q1,Q2,Q3,Q4,Q5
      COMMON/BLK3/B,B2,B3,C,AOO,BOO,EPSNU,OMEGA,C6
      COMMON/BLK4/CHSI10,CHSI20,ABARO,Z1BAR,LC
      COMMON/BLK7/ABC,COO,CO,OMEG1,P,R1,R2,TM,XNRHO
       COMMON/BLK8/ZOL,ZE,NG,TO,RAD,A
       COMMON/BLK10/CF1,CF2,CF4,QFO,RSTAR,ZL,L,SF1,SF2,AR,AAO,BBO
      COMMON/BLK22/AD,V1,V2,GG
      COMMON/BLK23/WO,ETAO,PTO,FRAC
      REAL K1,K2,K3,K4,K5,K6,K7,K8
       REAL LC,L
       WRITE(6,123)
123    FORMAT(1X,20H START OF PROGRAM          )
C      DEFAULT VALUES
      IEND=0
      ICOUNT=0
      NG=0
      FRAC=.018
       AR=2.
       TLE=39.0
       PTO=25.0
       WO=15.8
       ETAO=.38
       T=TLE+273.
      ZOL=7.50
       AAO=147.23
```

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```
      BBO=.0012
C     AAO,BBO USED IN LEAST SQ FIT OF SP.HEAT CONSTANT VOLUME
      P=40.
     LC=6.0
      XNRHO=1.0
     RAD=0.0
     COO=.5E25
      R1=.9975
      R2=.975
      ZE=5.0
     A=1.0
      TM= 1-R2
      OMEG1=5000.
      CON=2.0E4
     NAMELIST/PARAM/PTO,OMEG1,CON,COO,R1,R2,TM,XNRHO,LC,ZOL,A,ZE,
    1  AR, IEND ,FRAC ,T,PTO,RAD
C       ASSUME PRESSURE PTO (TORR) AND TEMPERATURE T (DEG K)
C       ARE GIVEN FOR LEFT END.  CALCULATE ETAO TO SATISFY GAS LAW
55    CONTINUE
     IF(IEND .EQ. 1) GO TO 600
     IF(NG.EQ.8) GO TO 600
      ICOUNT=ICOUNT+1
      READ(5,PARAM)
      IF(EOF(5))600,601
600   WRITE(6,603)
603   FORMAT(1X,28HEND OF FILE ENCOUNTERED-STOP)
      CALL PSEUDO
      DO 10 JJJ=1,5
      CALL GRAPHS(JJJ)
10    CONTINUE
      STOP 1313
C       P=PRESSURE, TORR
C     AR=LASER BEAM DIAMETER CM
C       A=RADIUS OF TUBE (CM)
C       RAD=RADIUS OF TUBE WHERE CALCULATIONS ARE DONE.
C       T=TEMPERATURE DEG K
C       TO=TEMPERATURE LEFT END DEG K
C     PTO= PRESSURE TORR LEFT END
C     WO=FLOW RATE LEFT END M/SEC
C     ETAO=DENSITY OF GAS KG/M**3
C       OMEG1=FLOW RATE, CM/SEC , MAXIMUM FLOW RATE AT RAD=0
C       CON=PEAK CONCENTRATION  , SOLAR CONSTANTS
```

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```
C       COO=INITIAL GUESS AT RHO-PLUS AT ZERO
C           WHICH IS SQUARE OF (COO*R1)
C       R1= REFLECTIVITY AT LEFT END
C       R2= REFLECTIVITY AT RIGHT END
C      ZE=DISTANCE FOR LIGHT INTENSITY TO DIMINISH BY FACTOR 1/E
C       TM= TRANSMISSION COEFFICIENT (OUTPUT MIRROR)
C      ZOL=POINT ALONG AXIS WHERE MAXIMUM ILLUMINATION OCCURS
C     IN THE CASE ILLUMINATION IS A BELL SHAPED CURVE
C      IN THE CASE OF A SQUARE WAVE, 2*ZOL IS CUT OFF POINT
C        THE POINT 2*ZOL IS WHERE ILLUMINATION BEGINS TO DIMINISH
C      LC=LENGTH OF CAVITY
C     ZL=2*ZOL     LENGTH WHICH IS ILLUMINATED
C      FRAC=FRACTION OF PEAK CONCENTRATION WHICH GOES
C            INTO HEAT
C           DEFAULT VALUEE IS FRAC=0.184 I.E. 1.84 PERCENT
C
601    CONTINUE
       P=PTO
       TO=T
       ETAO=P*(1.01325E5)*296./(8317.*760.*T)
C      ETAO IN KG/M**3
C      P IN TORR
C      T IN DEG K
       CMIN=1.0E10
       CMAX=1.0E30
      ZL=2*ZOL
       L=LC
       CO=CON
       C11=CON
      CALL COEFFS
C      WO IN M/SEC
       WO=OMEGA/100.
C      OMEG1 AND OMEGA ARE IN CM/SEC
       WRITE(6,198)
198    FORMAT(///)
      WRITE(6,199)  ZE,ZOL,CON,OMEGA,COO,R1,R2,P,T
199    FORMAT(1X, T5,5HZE = ,F10.3,T30,6HZOL = ,E15.7,T55,6HCON = ,
     1 E15.7,T80,8HOMEGA = ,E15.7,/,
     2 1X,T5,6HCOO = ,E15.7, T30,6H R1 = ,F10.7, T55,6H R2 = ,F10.7,
     3 T81,4H P = ,E15.7 ,T105,7HTEMP =  ,F10.3)
C     SET UP COEFFICIENTS IN DIFFERENTIAL EQUATIONS
C       SET PRINTER OFF
```

```
C        IPRINT=0        PRINTER OFF
C        IPRINT=1        PRINTER ON
         IPRINT=0
C        SET STEP SIZE H=1.0 CM
         H=1.0
C       INTEGRATE DIFFERENTIAL EQUATIONS FROM Z=0 TO Z=LC
        X1=C00
        CALL INTEG(IPRINT,H)
C
C          INTERVAL HALVING SCHEME
C
C         W1 AND W2 ARE WEIGHTS FOR INTERVAL HALVING SCHEME FOR
C         DETERMINING C00 WHICH SATISFIES BOUNDARY CONDITIONS
        Y1=ABC
         IF(Y1.LT.0) PER=.1
CC          IF(Y1.LT.0) PER=.9
         IF(Y1.GT.0) PER=10.
CC          IF(Y1.GT.0) PER=1.1
702      CONTINUE
         C00=(PER)*C00
         IF(C00 .LT. CMIN) STOP 5432
         IF(C00 .GT. CMAX) STOP 2345
        X2=C00
        CALL INTEG(IPRINT,H)
        Y2=ABC
         IF((Y1*Y2).LT. 0)GO  TO 701
         X1=C00
         Y1=Y2
         GO TO 702
701      CONTINUE
         W1=.4
         W2=.6
        C00=W2*X1+W1*X2
708     CONTINUE
         CALL INTEG(IPRINT,H)
         X3=C00
         Y3=ABC
         IF(ABS(Y3).LT.0.001) GO TO 555
704      CONTINUE
         IF((Y1*Y3).LT. 0) GO TO 705
C        Y1 & Y3 ARE OF THE SAME SIGN
         X1=X3
```

```
      Y1=Y3
      W3=ABS(2*Y1)+ABS(Y2)
      W1=ABS(2*Y1)/W3
      W2=ABS(Y2)/W3
      COO=W2*X1+W1*X2
      GO TO 708
  705 CONTINUE
C     Y1 & Y3 ARE OF OPPOSITE SIGN
      X2=X3
      Y2=Y3
      W3=ABS(2*Y1)+ABS(Y2)
      W1=ABS(2*Y1)/W3
      W2=ABS(Y2)/W3
      COO=W2*X1+W1*X2
      GO TO 708
  555  IPRINT=1
       H=0.25
       CALL INTEG(IPRINT,H)
       GO TO 55
     END
```

```
      SUBROUTINE GRAPHS(JJJ)
     COMMON/BLK4/CHSI10,CHSI20,ABARO,Z1BAR,LC
      COMMON/BLK8/ZOL,ZE,NG,TO,RAD,A
      COMMON/BLK30/DATA(1352,50),NDMAX,FLRATE(8)
      DIMENSION X(1352),Y(1352),YY(1352,8)
      REAL LC
C     JJJ=1,5
C     JJJ=1 PLOT R VS Z
C     JJJ=2 PLOT I2 VS Z
C     JJJ=3 PLOT I* VS Z
C     JJJ=4 PLOT I VS Z
C     JJJ=5 PLOT INV VS Z
C
C      DATA ARRAY IS BY COLUMNS
C      Z,R,I2,I*,I,INV,Z,R,I2,I*,I,INV,...
C      ND=NUMBER OF DATA POINTS,=NUMBER OF ROWS IN DATA ARRAY
C      NG=NUMBER OF CURVES PER GRAPH
C      IC IS CODE TO DETERMINE NUMBER OF GRAPHS TO PLOT
C      IC=0 FOR MORE THAN ONE GRAPH
C      IC=1 FOR LAST GRAPH (USED FOR ONLY ONE GRAPH)
C
       IC=0
       NLAST=NG-1
       IF(NLAST .EQ. 0) IC=1
C      PLOT JJJ VS Z
       DO 10 I=1,NDMAX
       X(I)=DATA(I,1)
       DO 20 J=1,NG
       NN=(J-1)*6
       NCOL=NN+1+JJJ
      YY(I,J)=DATA(I,NCOL)
20    CONTINUE
10    CONTINUE
C     FIND YMAX,YMIN
      DMAX=0.0
     YMAX=20.0
     YMIN=0.0
      ZMIN=0.0
C     PLOT FIRST DATA CURVE
C     JJJ=1
     BB=LC/10.
     IBB=1+INT(BB)
```

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```
      ZMAX=10.*IBB
       DO 40 I=1,NDMAX
      IF(ABS(YY(I,1)).LE. 1.0) GO TO 41
      Y(I)=(ALOG10(ABS(YY(I,1))) )*SIGN(1.0,YY(I,1))
      GO TO 40
 41   Y(I)=0.0
 40   CONTINUE
        ZMIN=0.0
        IF(JJJ.GT.1) GO TO 50
C       JJJ=1   PLOT R VS Z
        CALL INFOPLT(IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
     1  22,22HZ, AXIAL DISTANCE, CM     ,
     2  11,11HLOG [C3F7] ,0,
     3  10.,4.,1.5,1.5)
        GO TO 600
 50     CONTINUE
        IF(JJJ.GT.2) GO TO 100
C       JJJ=2   PLOT I2 VS Z
        CALL INFOPLT(IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
     1  23,23HZ, AXIAL DISTANCE, CM    ,
     2  9,9HLOG [I2]  ,0.,
     3  10.,4.,1.5,1.5)
      GO TO 600
 100  CONTINUE
      IF(JJJ.GT.3) GO TO 200
C     JJJ=3   PLOT I* VS Z
      CALL INFOPLT(IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
     1 23,23HZ, AXIAL DISTANCE, CM   ,
     2  9,9HLOG [I*]  ,0,
     3  10.,4.,1.5,1.5)
      GO TO 600
 200  CONTINUE
      IF(JJJ.GT.4) GO TO 300
C     JJJ=4    PLOT  I VS Z
      CALL INFOPLT(IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
     1  23,23HZ, AXIAL DISTANCE, CM   ,
     2  8,8HLOG [I]  ,0,
     3  10.,4.,1.5,1.5)
      GO TO 600
 300  CONTINUE
      YMIN=-20.0
C     JJJ=5   PLOT INV VS Z
```

```
              CALL INFOPLT(IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
             1  23,23HZ, AXIAL DISTANCE, CM  ,
             2  24,24H+,-LOG(ABS([I*]-.5*[I])) ,0,
             3  10.,4.0,1.5,1.5)
        600   CONTINUE
        C     PLOT REST OF CURVES OR EXIT IF ONLY ONE CURVE
               NLAST=NG-1
               IF(NLAST .EQ. 0) GO TO 601
               DO 500  J=2,NLAST
               DO 501 I=1,NDMAX
              IF(ABS(YY(I,J)) .LE. 1.0) GO TO 502
              Y(I)=(ALOG10(ABS(YY(I,J))) )*SIGN(1.0,YY(I,J))
              GO TO 501
        502   Y(I)=0.0
        501    CONTINUE
               CALL INFOPLT(IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
             1  1,1H   ,1,1H    , 0.,10.,4.,1.5,1.5)
        500    CONTINUE
        C      PLOT LAST CURVE
               DO 60 I=1,NDMAX
              IF(ABS(YY(I,NG)) .LE. 1.0) GO TO 61
              Y(I)=(ALOG10(ABS(YY(I,NG))) )*SIGN(1.0,YY(I,NG))
              GO TO 60
        61    Y(I)=0.0
        60    CONTINUE
              CALL INFOPLT(1,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
             1 1,1H  ,1,1H  ,0.,10.,4.,1.5,1.5)
        601      CONTINUE
              CALL NFRAME
              RETURN
              END
```

```
      SUBROUTINE PFLOW
C     SUBROUTINE TO CALCULATE THE PARAMETERS FOR SUBROUTINE FLOW
C     PARAMETERS STORE IN COMMON BLK10
     COMMON/BLK7/ABC,COO,CO,OMEG1,P,R1,R2,TM,XNRHO
     COMMON/BLK8/ZOL,ZE,NG,TO,RAD,A
      COMMON/BLK10/CF1,CF2,CF4,QFO,RSTAR,ZL,L,SF1,SF2,AR,AAO,BBO
     COMMON/BLK23/WO,ETAO,PTO,FRAC
     REAL L
C
C     AR IS BEAM DIAMETER RADIUS IN CM
      SF1=1000./296.
      SF2=(1.01325E5)/760.
C     SF1,SF2 ARE SCALE FACTORS FOR THE CORRECT UNITS OF
C     P=PRESSURE (N/M**2) , SF1 (MOLE/KG)
C     PT=PRESSURE (TORR),  SF2 (N/M**2)/TORR
C     ZL=LIGHT SOURCE LENGTH IN CM
C     ETA=DENSITY (KG/M**3)
C     L=TUBE LENGTH IN CM
C     RSTAR=GAS CONSTANT (JOULE/KG DEG K)
C     T=TEMPERATURE (DEG K)
C     CV=SPECIFIC HEAT AT CONSTANT VOLUME
C     W=FLOW VELOCITY (M/SEC) (SUBSCRIPTS O,L FOR START,END)
      PO=SF2*PTO
      RSTAR=8317.0/296.0
      CF1=ETAO*WO
      CF2=CF1*WO+PO
C     INTEGRAL OF CV(T)DT IS GIVEN BY
      XXX=BBO*(TO-300)
      CALL ETO(XXX,YYY)
      CVINTO=SF1*(AAO/BBO)*YYY
C     CONSTANTS CF4 AND QFO
      CF4=CF1*(RSTAR*TO+CVINTO)+CF1*WO*WO*.5
      QFO=FRAC*(1.35E3)*CO
      QFO=QFO*1.0/ZL
      RETURN
      END
```

```
      SUBROUTINE FLOW(Z,T,PTORR,W,ETA)
      COMMON/BLK8/ZOL,ZE,NG,TO,RAD,A
C     SUBROUTINE TO CALCULATE T,P,W,ETA AS FUNCTION OF Z
      COMMON/BLK10/CF1,CF2,CF4,QFO,RSTAR,ZL,L,SF1,SF2,AR,AAO,BBO
     COMMON/BLK23/WO,ETAO,PTO,FRAC
C
      COMMON/BLK29/ ZZZ,TZZ,PZZ,ETAZZ,WZZ
     REAL L
      ICOUNT=0
      Q=QFO*Z
C     ENERGY INPUT TERM DETERMINED BY QFO
      IF(Z.GT.ZL)     Q=QFO*ZL
     T=TO
 50   CONTINUE
     W=(CF2-SQRT(CF2*CF2-4.*CF1*CF1*RSTAR*T))/(2.*CF1)
     ETA=CF1/W
     XXX=BBO*(T-300)
     CALL ETO(XXX,YYY)
     P=ETA*RSTAR*T
     F=CF1*RSTAR*T+CF1*SF1*(AAO/BBO)*YYY+CF1*.5*W*W-Q-CF4
     FP=CF1*RSTAR+CF1*SF1*AAO*YYY+W*(ETA*RSTAR)/((P/W)-CF1)
     T1=T-F/FP
     ERROR=ABS(100*(T1-T)/T)
     IF(ERROR .LT. 1.0) GO TO 100
     T=T1
      ICOUNT=ICOUNT+1
      IF(ICOUNT .GT. 100) STOP 4444
     GO TO 50
 100 CONTINUE
     T=T1
     W=(CF2-SQRT(CF2*CF2-4.*CF1*CF1*RSTAR*T))/(2.*CF1)
     TC=T-273
      ETA=CF1/W
      PNM2=ETA*RSTAR*T
      PTORR=PNM2/SF2
     ZZZ=Z
     TZZ=TC
     PZZ=PTORR
     ETAZZ=ETA
     WZZ=W
      RETURN
      END
```

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```
      SUBROUTINE ARREN(TEMP)
C     SUBROUTINE FOR ARRENHIUS EXPRESSION OF RATE COEFFICIENTS
C     BASIC ASSUMPTIONS
C      FOR QI TERMS QI=QIO*EXP(-BETA*(TEMP-TO))
C      TREAT KI TERMS LIKE CI TERMS
C
     COMMON/BLK2/K1,K2,K3,K4,K5,K6,K7,K8,C1,C2,C3,C4,C5
     COMMON/BLK27/Q1,Q2,Q3,Q4,Q5
     COMMON/BLK3/B,B2,B3,C,A00,B00,EPSNU,OMEGA,C6
      COMMON/BLK11/KK1,KK2,KK3,KK4,KK5,KK6,KK7,KK8
      COMMON/BLK12/QQ1,QQ2,QQ3,QQ4,QQ5
     COMMON/BLK13/CC1,CC2,CC3,CC4,CC5,CC6
      REAL K1,K2,K3,K4,K5,K6,K7,K8,KK1,KK2,KK3,KK4,KK5,KK6,KK7,KK8
C
C      REFERENCE J.S. COHEN AND U.P. JUDD
C              J.APPL. PHYS., VOL 55, NO. 7, APRIL 1984
C      COEFFICIENTS MODIFIED TO ACHIEVE SPECIFIC VALUES AT TEMPERATURE
C      OF 276 DEGREES K.
C
       BETA=4.4E-3
       SF1=1.0
      XXX=-BETA*(TEMP-300)
      CALL ETO(XXX,YYY)
       SF2=YYY
       K1=KK1*SF1
       K2=KK2*SF1
       K3=KK3*SF1
       K4=KK4*SF1
       K5=KK5*SF1
       K6=KK6*SF1
       K7=KK7*SF1
       K8=KK8*SF1
     C1=CC1*SF1
     C2=CC2*EXP(1205.76/TEMP)
     C3=CC3*SF1
      XYZ=-29.5207-5.844*ALOG(TEMP/300.)+2.163*(ALOG(TEMP/300.))**2
      C4=10.0**XYZ
      C5=CC5*EXP(1191.626/TEMP)
     C6=CC6*SF1
      Q1=QQ1*SF1
      Q2=QQ2*EXP(-4.4E-3*(TEMP-300))
      Q3=QQ3*SF1
```

```
SUBROUTINE ARREN      74/860  OPT=1  PMDMP                FTN 4.8+688       88/11/02. 14.55.42       PAGE    2

              Q4=QQ4*SF1
              Q5=QQ5*SF1
              RETURN
              END
```

```
FUNCTION CHSI1        74/860  OPT=1  PMDMP                FTN 4.8+688       88/11/02. 14.55.42       PAGE    1

              FUNCTION CHSI1(Z)
C             IMPLICIT REAL*8(A-H,K,L,O-Z)
              COMMON/BLK4/CHSI10,CHSI20,ABARO,Z1BAR,LC
              COMMON/BLK8/ZOL,ZE,NG,TO,RAD,A
              REAL LC
              IF(Z.LT.ABARO) GO TO 100
              IF(Z.LT.Z1BAR) GO TO 200
C             Z GREATER THAN Z1BAR
100           CHSI1=0.0
C              CHSI1 HAS UNITS OF SEC^-1
              RETURN
200           CONTINUE
              CHSI1=CHSI10
              RETURN
              END
```

```
SUBROUTINE ETO        74/860  OPT=1  PMDMP                FTN 4.8+688       88/11/02. 14.55.42       PAGE    1

              SUBROUTINE ETO(X,Y)
              IF(X .LT. -670.) GO TO 100
              Y=EXP(X)
              RETURN
100           Y=0.
              RETURN
              END
```

FUNCTION CHSI2   74/860 OPT=1 PMDMP   FTN 4.8+688   88/11/02. 14.55.42   PAGE 1

```
C
      FUNCTION CHSI2(Z)
C     IMPLICIT REAL*8(A-H,K,L,O-Z)
      COMMON/BLK4/CHSI10,CHSI20,ABARO,Z1BAR,LC
      COMMON/BLK8/ZOL,ZE,NG,TO,RAD,A
      REAL LC
      IF(Z.LT.ABARO) GO TO 100
      IF(Z.LT.Z1BAR) GO TO 200
C     Z GREATER THAN Z1BAR
       XXX=-(Z-Z1BAR)/ZE
       CALL ETO(XXX,YYY)
      CHSI2=CHSI20*YYY
C     CHSI2 HAS UNITS OF SEC^-1
      RETURN
100   CHSI2=0.0
      RETURN
200   CONTINUE
      CHSI2=CHSI20
      RETURN
      END
```

SUBROUTINE VELOC   74/860 OPT=1 PMDMP   FTN 4.8+688   88/11/02. 14.55.42   PAGE 1

```
C
      SUBROUTINE VELOC(OMEG1,RAD,OMEGA,A)
C     CALCULATE VELOCITY OMEGA AT R=RAD
C          0 .LE. RAD  .LE. A
C
C     TYPE OF FLOW
      OMEGA=(OMEG1/(A*A))*(RAD-A)**2
      RETURN
      END
```

```
C
      SUBROUTINE COEFFS
C       THIS SUBROUTINE DEFINES THE COEFFICIENTS IN THE DIFFERENTIAL
C       EQUATIONS TO BE SOLVED.
C     IMPLICIT REAL*8(A-H,K,L,O-Z)
      COMMON/BLK22/AD,V1,V2,GG
      COMMON/BLK3/B,B2,B3,C,A00,B00,EPSNU,OMEGA,C6
      COMMON/BLK4/CHSI10,CHSI20,ABARO,Z1BAR,LC
      COMMON/BLK7/ABC,C00,CO,OMEG1,P,R1,R2,TM,XNRHO
       COMMON/BLK8/ZOL,ZE,NG,TO,RAD,A
       COMMON/BLK11/KK1,KK2,KK3,KK4,KK5,KK6,KK7,KK8
       COMMON/BLK12/QQ1,QQ2,QQ3,QQ4,QQ5
      COMMON/BLK13/CC1,CC2,CC3,CC4,CC5,CC6
      REAL KK1,KK2,KK3,KK4,KK5,KK6,KK7,KK8,LC
C
C     COEFFICIENTS IN THE DIFFERENTIAL EQUATIONS
C
      OMEGA=OMEG1
       CALL VELOC(OMEG1,RAD,OMEGA,A)
      ABARO=0.0
C      ABARO= START OF ILLUMINATION
C       Z1BAR=2*ZOL = POINT ON AXIS WHERE ILLUMINATION BEGINS TO DIMINISH
      CHSI10=(3.04E-3)*CO*XNRHO
C       COO IS THE CONCENTRATION IF SOLAR CONSTANTS
      CHSI20=(3.38E-2)*CO
      Z1BAR=2*ZOL
      EPSNU=1.5E-19
C      WATTS*SEC
      A00=2.0E17
      B00=.443
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C       (CHSI1)    HV + RI --> R + I*
C       (CHSI2)    HV + I2 --> I* + I     (51% OF THE TIME)
C       (CHSI2)    HV + I2 -->  I + I    (49% OF THE TIME)
CC         (KK1)     I* + R --> RI
CC         (KK2)     I + R --> RI
CC         (KK3)     R + R --> R2
CC         (KK4)     R + RI --> R2 + I
CC         (KK5)     R + I2 --> RI + I
CC         (KK6)     R + RI --> R2 + I*
```

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```
CC          (KK7)      I* + RI --> I2 + R
CC          (KK8)      I + RI --> I2 + R
CC
CC          (QQ1)      I* + RI --> I + RI
CC          (QQ2)      I* + I2 --> I + I2
CC          (QQ3)      I* + R --> I + R
CC          (QQ4)      I* + R2 --> I + R2
CC          (QQ5)      I* + I --> I + I
CC
CC          (CC1)      I* + I + RI --> I2 + R1
CC          (CC2)      I + I + RI --> I2 + RI
CC          (CC3)      I* + I + I2 --> I2 + I2
CC          (CC4)      I + I + I2 --> I2 + I2
CC          (CC5)      I + I + R2 --> I2 + R2
CC          (CC6)      I + I* + R2 --> I2 + R2
CC
CC
CC        WALL REACCTIONS
CC
CC          (V1)      I + I + WALL --> I2 + WALL
CC          (V2)     R2 + I + WALL --> R + RI + WALL
CC
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
CC
CC       KK1 = 34.7E-13
CC       KK1 = 5.6E-13
        KK1 = .9E-13
CC
        KK2 = 8.05E-11
CC       KK2 = 2.3E-11
CC       KK2 = .657E-11
CC
CC       KK3 = 10.4E-12
CC       KK3 = 2.6E-12
        KK3 = .26E-11
CC
CC       KK4 =      9.E-16
CC       KK4 = 3.E-16
        KK4 =      1.E-16
CC
        KK5 =     3.E-11
CC       KK5 = 1.0E-11
```

```
CC     KK5 =      .33E-11
CC
      KK6 = 10.24E-17
CC     KK6 = 3.2E-17
CC     KK6 = 1.E-17
CC
CC     KK7 = 4.5E-19
CC     KK7 = 3.0E-19
      KK7 = 1.5E-19
CC
CC     KK8 =       4.8E-23
CC     KK8 = 1.6E-23
CC     KK8 =       .533E-23
      KK8 = 0.0
CC
CC     QQ1 = 8.4E-16
CC     QQ1 = 2.0E-16
      QQ1 = .476E-16
CC
CC     QQ2 = 4.94E-11
CC     QQ2 = 1.9E-11
      QQ2 = .65868E-11
CC
CC     QQ3 =       11.1E-18
CC     QQ3 = 3.7E-18
      QQ3 =     1.23E-18
CC
CC     QQ4 =      14.1E-16
CC     QQ4 = 4.7E-16
      QQ4 =     1.57E-16
CC
CC     QQ5 =      4.8E-14
CC     QQ5 = 1.6E-14
      QQ5 =      .53E-14
CC
CC     CC1 = 10.2E-33
CC     CC1 = 3.2E-33
      CC1 = 1.E-33
CC
      CC2 = 5.7E-33
CC     CC2 = 8.5E-32
CC     CC2 = 1.6E-32
```

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```
CC
CC     CC3 = 14.4E-32
CC     CC3 = 8.E-32
      CC3 = 4.44E-32
CC
      CC4 = 4.94E-30
CC     CC4 = 3.8E-30
CC     CC4 = 2.92E-30
CC
CC     CC5 = 6.E-31
      CC5 = 8.0E-33
CC     CC5 = 3.6E-31
CC
CC     CC6 =       2.25E-32
CC     CC6 =       1.8E-32
CC     CC6 =       1.35E-32
      CC6 = 0.0
CC
C     V1 =       3.0E-12
C     V1 =       1.0E-12
C     V1 =       .33E-12
      V1 = 0.0
C
C     V2 =       3.0E-11
C     V2 =       1.0E-11
C     V2 =        .33E-11
      V2 = 0.0
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C     KK1=.903E-13
C     KK2=80.E-12
C     KK3=.65E-12
C     KK4=1.000E-16
C     KK5=3.009E-11
C     KK6=1.0E-17
C     KK7=.1517E-18
C     KK8=1.6E-23
C
C     QQ1=.476E-16
C     QQ2=1.9E-11
C     QQ3=.1235E-17
```

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```
C       QQ4=1.57E-16
C       QQ5=.53E-14
C
CC       CC1=1.053E-33
CC       CC2=45.0E-32
CC       CC3=.4447E-31
CC       CC4=4.94E-30
CC       CC5=3.6E-31
CC       CC6=      1.8E-32
C
C       V1=       1.0E-12
C       V2=       1.0E-11
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
        GG=2*(.18/LC)**2
        C=3.0E10
        B=(9.66E18)*P/T0
        B2=B*B
        B3=B2*B
CC         WRITE OUT CCOEFFICCIENTS
         WRITE(6,100) KK1,KK7,QQ1,CC5
         WRITE(6,101) KK2,KK8,QQ2,V1
         WRITE(6,102) KK3,CC1,QQ3,V2
         WRITE(6,103) KK4,CC2,QQ4,RAD
         WRITE(6,104) KK5,CC3,QQ5,A
         WRITE(6,105) KK6,CC4,CC6
100      FORMAT(T5,5HKK1 = ,E15.7,T30,5HKK7 = ,E15.7,T60,5HQQ1 = ,E15.7 ,
       1 T85,5HCC5 =  , E15.7 )
101      FORMAT(T5,5HKK2 = ,E15.7,T30,5HKK8 = ,E15.7,T60,5HQQ2 = ,E15.7 ,
       1 T85,5HV1 =   , E15.7 )
102      FORMAT(T5,5HKK3 = ,E15.7,T30,5HCC1 = ,E15.7,T60,5HQQ3 = ,E15.7 ,
       1  T85, 5HV2 =  , E15.7)
103      FORMAT(T5,5HKK4 = ,E15.7,T30,5HCC2 = ,E15.7,T60,5HQQ4 = ,E15.7,
       1 T85, 6HRAD = ,F10.4 )
104      FORMAT(T5,5HKK5 = ,E15.7,T30,5HCC3= ,E15.7,T60,5HQQ5 = ,E15.7,
       1 T85, 6H A  =  ,F10.4 )
105      FORMAT(T5,5HKK6 = ,E15.7,T30,5HCC4= ,E15.7,T60,5HCC6 = ,E15.7 )
        RETURN
        END
```

```
      SUBROUTINE FUN(N,Z,Y,F)
C       THIS SUBROUTINE DEFINES THE RIGHT HAND SIDE
C       OF THE DIFFERENTIAL EQUATIONS FOR THE CHEMICAL KINETICS
C     IMPLICIT REAL*8(A-H,K,L,O-Z)
      DIMENSION Y(7),F(7)
      COMMON/BLK1/X7,POWER
      EXTERNAL CHSI1,CHSI2
      COMMON/BLK2/K1,K2,K3,K4,K5,K6,K7,K8,C1,C2,C3,C4,C5
      COMMON/BLK27/Q1,Q2,Q3,Q4,Q5
      COMMON/BLK3/B,B2,B3,C,A00,B00,EPSNU,OMEGA,C6
      COMMON/BLK4/CHSI10,CHSI20,ABAR0,Z1BAR,LC
      COMMON/BLK7/ABC,C00,C0,OMEG1,P,R1,R2,TM,XNRHO
      COMMON/BLK22/AD,V1,V2,GG
      REAL K1,K2,K3,K4,K5,K6,K7,K8,LC
C
C     QY=QUANTUM YIELD
      QY=1.0
C
C       F(I),I=1,6 ARE RATES OF CHANGES FOR THE CONCENTRATIONS
C        F(1)=D[RI]/DZ                F(2)=D[R]/DZ
C        F(3)=D[R2]/DZ                F(4)=D[I2]/DZ
C        F(5)=D[I*]/DZ                F(6)=D[I]/DZ
C
20    CONTINUE
C      Z IS DISTANCE IN CM
C      CALCULATE GAS PARAMETERS AS FUNCTION OF Z
C      CALL FLOW(Z,TEMP,PRESS,FLOWR,DENSITY)
       CALL FLOW(Z,TEMP,PRESS,FLOWR,DENSITY)
C      TEMP IS TEMPERATURE DEG K
C      PRESS IS PRESSURE IN TORR
C      FLOWR IS FLOWRATE IN M/SEC
C      DENSITY IS GAS DENSITY IN KG/M**3
       OMEGA=FLOWR*100.
C      OMEGA IS FLOW RATE IN CM/SEC
C      CALCULATE COEFFICIENTS AS FUNCTION OF TEMP AND Z
       CALL ARREN(TEMP)
C      CONSTANTS COME VIA COMMON BLKS 2 AND 3
C      K'S IN CM**3/SEC
C      C'S IN CM**6/SEC
C      Q'S IN CM**3/SEC
C      POWER IS IN W/CM**2
       X8=C00/(Y(7)*B)
```

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```
      X7STAR=Y(7)*B+X6
      DIF=Y(5)-.5*Y(6)
      CALL SIGMA(SIG2)
      SIG=SIG2
     F(1)=K1*B*Y(2)*Y(5)+K2*B*Y(2)*Y(6)-CHSI1(Z)*Y(1)-K4*B*Y(1)*Y(2)
    1 +K5*B*Y(2)*Y(4) -K7*B*Y(5)*Y(1)-K6*B*Y(2)*Y(1)  +V2*B*Y(3)*Y(6)
    2  -K8*B*Y(6)*Y(1)
     F(2)=CHSI1(Z)*Y(1)-K1*B*Y(2)*Y(5)-K2*B*Y(2)*Y(6)-2*K3*B*Y(2)*Y(2)
    1 -K4*B*Y(1)*Y(2)-K6*B*Y(1)*Y(2)-K5*B*Y(2)*Y(4)+V2*B*Y(3)*Y(6)
    2 +K7*B*Y(5)*Y(1) +K8*B*Y(6)*Y(1)
     F(3)=K3*B*Y(2)*Y(2)+K6*B*Y(1)*Y(2)+K4*B*Y(1)*Y(2)-V2*B*Y(3)*Y(6)
     A1=C1*B2*Y(1)*Y(5)*Y(6)+C2*B2*Y(1)*Y(6)*Y(6)+C3*B2*Y(4)*Y(5)*Y(6)
     A2=C4*B2*Y(4)*Y(6)*Y(6)-CHSI2(Z)*Y(4)+K7*B*Y(5)*Y(1)
    1 -K5*B*Y(2)*Y(4) +V1*B*Y(6)*Y(6) +C5*B2*Y(6)*Y(6)*Y(3)
     F(4)=A1+A2 +K8*B*Y(6)*Y(1) +C6*B2*Y(6)*Y(5)*Y(3)
     A3=QY*CHSI1(Z)*Y(1)+0.51*CHSI2(Z)*Y(4)-K1*B*Y(2)*Y(5)
     A4=-C1*B2*Y(1)*Y(5)*Y(6)-C3*B2*Y(4)*Y(5)*Y(6)-Q1*B*Y(1)*Y(5)
     A5=-Q2*B*Y(4)*Y(5)-C*SIG*X7STAR*DIF +K6*B*Y(2)*Y(1)
     F(5)=A3+A4+A5-Q3*B*Y(5)*Y(2)-Q4*B*Y(5)*Y(3)-Q5*B*Y(5)*Y(6)
    1 -K7*B*Y(5)*Y(1)  -C6*B2*Y(6)*Y(5)*Y(3)
     A6=1.49*CHSI2(Z)*Y(4)+Q1*B*Y(1)*Y(5)+Q2*B*Y(4)*Y(5)
    1  -2*C5*B2*Y(6)*Y(6)*Y(3)  -K8*B*Y(6)*Y(1)
     A7=C*SIG*X7STAR*DIF -C1*B2*Y(1)*Y(5)*Y(6)
     A8=-2*C2*B2*Y(1)*Y(6)*Y(6)-C3*B2*Y(4)*Y(5)*Y(6)
     A9=-2*C4*B2*Y(4)*Y(6)*Y(6)-K2*B*Y(2)*Y(6)+K4*B*Y(1)*Y(2)
      A10=Q3*B*Y(5)*Y(2)+Q4*B*Y(5)*Y(3)+Q5*B*Y(5)*Y(6)
    1 +K5*B*Y(2)*Y(4)  -V2*B*Y(3)*Y(6) -2*V1*B*Y(6)*Y(6)
     F(6)=A6+A7+A8+A9+A10 -C6*B2*Y(6)*Y(5)*Y(3)
     DO 10 I=1,6
  10 F(I)=F(I)/OMEGA
      F(7)=Y(7)*DIF*B*SIG
     RETURN
     END
```

```
C
       SUBROUTINE SIGMA(SIG)
C      THIS SUBROUTINE DEFINES THE CROSS SECTION SIGMA
      COMMON/BLK3/B,B2,B3,C,A00,B00,EPSNU,OMEGA,C6
      COMMON/BLK7/ABC,C00,C0,OMEG1,P,R1,R2,TM,XNRHO
       REAL NU,NUS,NU0,NU1,NU2,NU3,NU4 ,NU5
       PI=3.14159
       PIS=PI*PI
       NU=C/1.315246E-4
       NUS=NU*NU
       PISNUS=PIS*NUS*4.
       G=0
       CS=C*C
       NU0=NU
       NU1=NU0+.141*C
       NU2=NU1+.068*C
       NU3=NU0-.427*C
       NU4=NU3-.026*C
       NU5=NU4-.068*C
       DELTA23=NU-NU5
       DELTA22=NU-NU4
       DELTA21=NU-NU3
       DELTA34=NU-NU0
       DELTA33=NU-NU1
       DELTA32=NU-NU2
       TEMPO=293
       TWALL=TEMPO
       T1=TWALL
       A=5.434
       A1=A*2.4/7.7*CS
       A2=A*3.0/7.7*CS
       A3=A*2.3/7.7*CS
       A4=A*5.0/7.7*CS
       A5=A*2.2/7.7*CS
       A6=A*0.6/7.7*CS
       FUGTEMP=SQRT(T1/300.)
       ALPHAM=1.88E7*FUGTEMP
       DELDOP=2.51E8*FUGTEMP
       DELNU=DELDOP+ALPHAM*P
       SIGMA23=A1/(PISNUS*DELNU)/(1+(2.*DELTA23/DELNU)**2)*5./12.
       SIGMA22=A2/(PISNUS*DELNU)/(1+(2.*DELTA22/DELNU)**2)*5./12.
       SIGMA21=A3/(PISNUS*DELNU)/(1+(2.*DELTA21/DELNU)**2)*5./12.
```



```
       SIGMA34=A4/(PISNUS*DELNU)/(1+(2.*DELTA34/DELNU)**2)*7./12.
       SIGMA33=A5/(PISNUS*DELNU)/(1+(2.*DELTA33/DELNU)**2)*7./12.
       SIGMA32=A6/(PISNUS*DELNU)/(1+(2.*DELTA32/DELNU)**2)*7./12.
       SIGMAT=SIGMA23+SIGMA22+SIGMA21+SIGMA34+SIGMA33+SIGMA32
       SIG=SIGMAT
       RETURN
       END
```

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```
      C
            SUBROUTINE INTEG(IPRINT,H)
      C      THIS SUBROUTINE INTEGRATES THE SYSTEM OF DIFFERENTIAL EQUATIONS
      C      USING A VARIABLE STEP SIZE 7TH ORDER RUNGE KUTTA-FEHLBERG METHOD.
      C     IMPLICIT REAL*8(A-H,K,L,O-Z)
            DIMENSION YO(7),X(7),WK(49)
            COMMON/BLK1/X7,POWER
            COMMON/BLK3/B,B2,B3,C,A00,B00,EPSNU,OMEGA,C6
            COMMON/BLK4/CHSI10,CHSI20,ABARO,Z1BAR,LC
            COMMON/BLK7/ABC,C00,CO,OMEG1,P,R1,R2,TM,XNRHO
             COMMON/BLK8/ZUL,ZE,NG,TO,RAD,A
            COMMON/BLK22/AD,V1,V2,GG
            COMMON/BLK29/ZZZ,TZZ,PZZ,ETAZZ,WZZ
            COMMON/BLK30/DATA(1352,50),NDMAX,FLRATE(8)
            EXTERNAL FUN,CHSI1,CHSI2
            REAL LC
      C
      C     INTEGRATE SYSTEM FROM Z=0 TO Z=LC USING RUNGE-KUTTA METHOD
      C
      C     X(1)=RI
      C     X(2)=R
      C     X(3)=R2
      C     X(4)=I2
      C     X(5)=I*
      C     X(6)=I
      C     X(7)=RHO+
      C     X8=RHO-
      C     X9=I*-.5*I
      C
             WW2=(.98)**2
      C     INITIALIZE CONSTANTS FOR FLOW EQUATIONS
      C     SEE COMMON BLK10 FOR THESE CONSTANTS--NEEDED FOR SUB FLOW
            CALL PFLOW
            ND=0
      C       TEST FOR PRINT CONDITIONS
             IF(IPRINT.EQ. 0) GO TO 229
             NG=NG+1
            FLRATE(NG)=OMEGA
             WRITE(8,331) LC
       331    FORMAT(1X,11H   LC     =  ,F10.2)
       229     CONTINUE
       55     CONTINUE
```

```
      N=7
      TOL=1.0E-6
      PD=1.0
      MTH=1
C      H IS STEP SIZE IN CM BETWEEN PRINT OUTS
C      IPRINT=0 OFF, IPRINT=1 ON
       HMIN=H/10000000.
       HMAX=H/100.
       HUSE=HMIN*10
       IERR=0
C     INITIAL CONDITIONS
      Z0=0.0
      YO(1)=1.0
       Z1=0.0
      DO 9 I=2,6
9     YO(I)=0.0
C       GUESS AT INITIAL CONDITIONS FOR X(7) AND X(8)
       X70=SQRT(R1*COO)
       YO(7)=X70/B
       IF(IPRINT .EQ. 0) GO TO  300
       WRITE(6,191)
191   FORMAT(///,T7,1HZ,T20,4H[RI],T32,4H[R],T45,5H[R2],T57,4H[I2],
     1 T69,4H[I*],T80,4H[I] ,T91,6H[RHO+],T103,6H[RHO-],T112,
     2 9HINVERSION        )
300   CONTINUE
C     PRINT OUT
      DO 10 I=1,7
10    X(I)=B*YO(I)
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C       USE CONSERVATION LAWS---THE ABOVE SYSTEM OF DIFFERENTIAL
C       EQUATIONS HAS THE TWO INTEGRALS
C
C           [RI] + [R] +2[R2] = CONSTANT= B
C      OR
C            Y(1) + Y(2) + 2Y(3)= 1.0
C
C    AND    [RI]  + 2[I2] + [I*] + [I] = B
C      OR
C             Y(1) + 2Y(4) + Y(5) + Y(6) =1.0
C
```

```
      YOTH2=1.0-YO(1)-2.*YO(3)
      YOTH6=1.0-YO(5)-2.0*YO(4)-YO(1)
C     TEST TO SEE IF YOTH2 IS ZERO
      ERROR1=0.0
      IF(YOTH2.EQ.0.0 ) GO TO 1555
      ERROR1=(YO(2)-YOTH2)*100/YOTH2
1555    CONTINUE
      ERROR2=0.0
C     TEST TO SEE IF YOTH6 IS ZERO
      IF(YOTH6.EQ. 0.0) GO TO 1556
      ERROR2=(YO(6)-YOTH6)*100/YOTH6
1556    CONTINUE
      IF((ERROR1.OR. ERROR2).GT. .5) WRITE(6,1222)
1222  FORMAT(1X, 40H ERROR1 OR ERROR2 IS OUT OF BOUNDS      )
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C   END OF TEST FOR CONSERVATION LAWS BEING SATISFIED
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      X8=C00/X(7)
     X9=X(5)-.5*X(6)
      X7STAR=X(7)+X8
C      USE SUBROUTINE SIGMA TO CALCULATE CROSS SECTION SIGMA
     CALL SIGMA(SIG2)
      IF(IPRINT .EQ. 0) GO TO 222
     WRITE(6,199)Z0,(X(I),I=1,7),X8,X9
222    CONTINUE
      IF(IPRINT .EQ. 0) GO TO 227
      ICOL=(NG-1)*6
      ND=ND+1
      DATA(ND,ICOL+2)=X(2)
      DATA(ND,ICOL+1)=Z0
      DATA(ND,ICOL+3)=X(4)
      DATA(ND,ICOL+4)=X(5)
      DATA(ND,ICOL+5)=X(6)
      DATA(ND,ICOL+6)=X9
C     WRITE Z,R,12,I*,1,INV
      WRITE(8,6773) Z0,X(2),X(4),X(5),X(6),X9
6773  FORMAT(1X,F6.2,2X,5(2X,E15.4))
227   CONTINUE
     IF(Z0.LE.0.0) GO TO 3567
```

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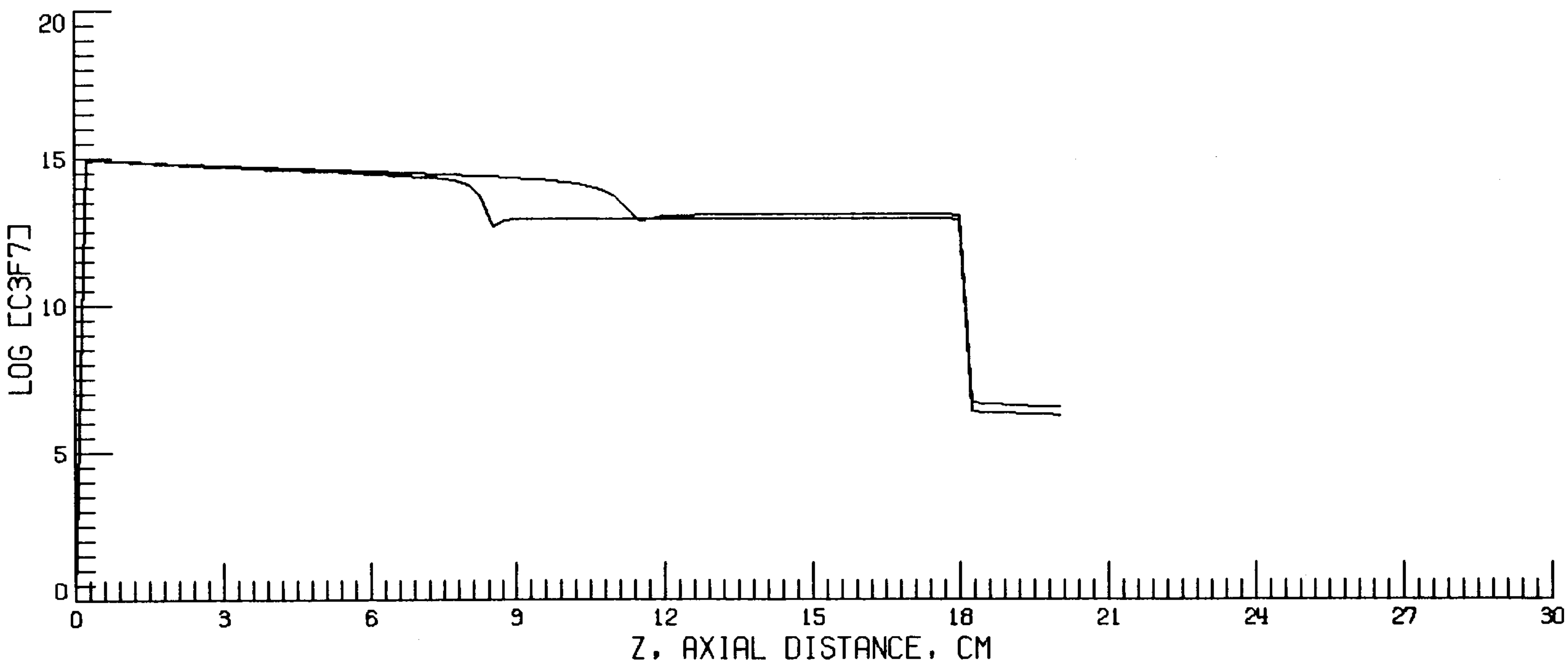
```
                IF(IPRINT .EQ. 0) GO TO 223
                WRITE(6,303)ZZZ,TZZ,PZZ,ETAZZ,WZZ
       223        CONTINUE
       303      FORMAT(1X,T2,3HZ= ,F5.2,2X,T15,3HT= ,F7.3,2X,T30,
              1 7HPTORR=  ,F9.2,2X,
              2 T55,9HDENSITY = ,F9.6,2X,T80,3HW=  ,F7.2   )
      3567       CONTINUE
       199     FORMAT(1X,E12.5,8E12.5,E12.5 ,E12.5  )
       C
       C          USE 7TH ORDER RUNGE KUTTA INTEGRATION SCHEME WITH VARIABLE STEP
       C           STEP SIZE CAN VARY FROM HMIN TO HMAX
       C           Z0 IS STARTING VALUE FOR Z
       C           Z1 IS NEXT STOPPING POINT IN INTEGRATION SCHEME
       C           TOL IS TOLERENCE
       C           IERR IS ERROR CODE TO DETERMINE IF INTEGRATION WAS SUCCESSFUL
       C         IF INVERSION DENSITY HAS GONE NEG JUMP OUT OF LOOP
       C         IF  (X9.LE.(-.1E-1)) GO TO 111
       C
       100     CONTINUE
                Z1=Z1+H
                CALL RKF7(N,Z0,Z1,Y0,TOL,FUN,PD,MTH,HMIN,HMAX,HUSE,WK,IERR)
                IF(IERR .NE. 0)  WRITE(6,444)
               IF(IERR .NE. 0) STOP 1717
       444     FORMAT(1X,35H IERR IS NOT ZERO                              )
       200     CONTINUE
                X(7)=B*Y0(7)
                X8=C00/X(7)
       60      FORMAT(1X,5(2X,E14.6))
               IF((Z1+.5*H).GE.(LC+.2)) GO TO 111
       CC         IF(X(7) .GT. X8) GO TO 237
               GO TO 300
       500     CONTINUE
                DO 110 I=1,7
       110      X(I)=B*Y0(I)
                X8=C00/X(7)
                 X9=X(5)-.5*X(6)
       111       CONTINUE
                 XX7L=B*Y0(7)
                RHOPL=X70/(SQRT(R2*R1))
                DO 112 I=1,7
       112      X(I)=B*Y0(I)
                X8=C00/X(7)
```

```
           X9=X(5)-.5*X(6)
           IF(IPRINT .EQ. 0) GO TO 224
          WRITE(6,199)ZO,(X(I),I=1,7),X8,X9
  224      CONTINUE
  C        RHOPL=RHO-PLUS AT Z=L THEORETICAL VALUE
  C        XX7L= CALCULATED VALUE OF RHO-PLUS AT Z=
  C        ABC =DIFFERENCE=XX7L-RHOPL
           DIF=(((XX7L-RHOPL)/RHOPL)*100)
           ABC=DIF
           IF(IPRINT .EQ. 0) GO TO 225
          WRITE(6,202)DIF,RHOPL,XX7L,COO
  225        CONTINUE
  202     FORMAT(1X,13HDIFFERENCE = ,E18.9,2X,12HTHEORETICAL=,E18.9,2X,
         1 10H ACTUAL = , E18.9,2X,6HCOO =    ,E18.8 )
  237      CONTINUE
  C
          XX7L=X(7)
  CC       TM=1-R2/(WW2)
  CC       IF(TM .LT. 0) GO TO 300
           POWER=EPSNU*TM*C*XX7L
           IF(IPRINT .EQ. 0) GO TO 226
           WRITE(6,193)R1,R2,POWER,TM,ZO,P
  226        CONTINUE
  193     FORMAT(1X,5HR1 = ,F10.7,1X,5HR2 = ,F10.7,1X,7HPOWER = ,E18.10,
         1 1X,5HTM = ,F10.8,1X,4HL = ,F15.7 ,2X,4HP = ,F15.7 )
          IF((Z1+.5*H).GE.(LC+.2)) GO TO 501
          GO TO 300
  501      CONTINUE
           NDMAX=ND
          RETURN
          END
```

A P P E N D I X B



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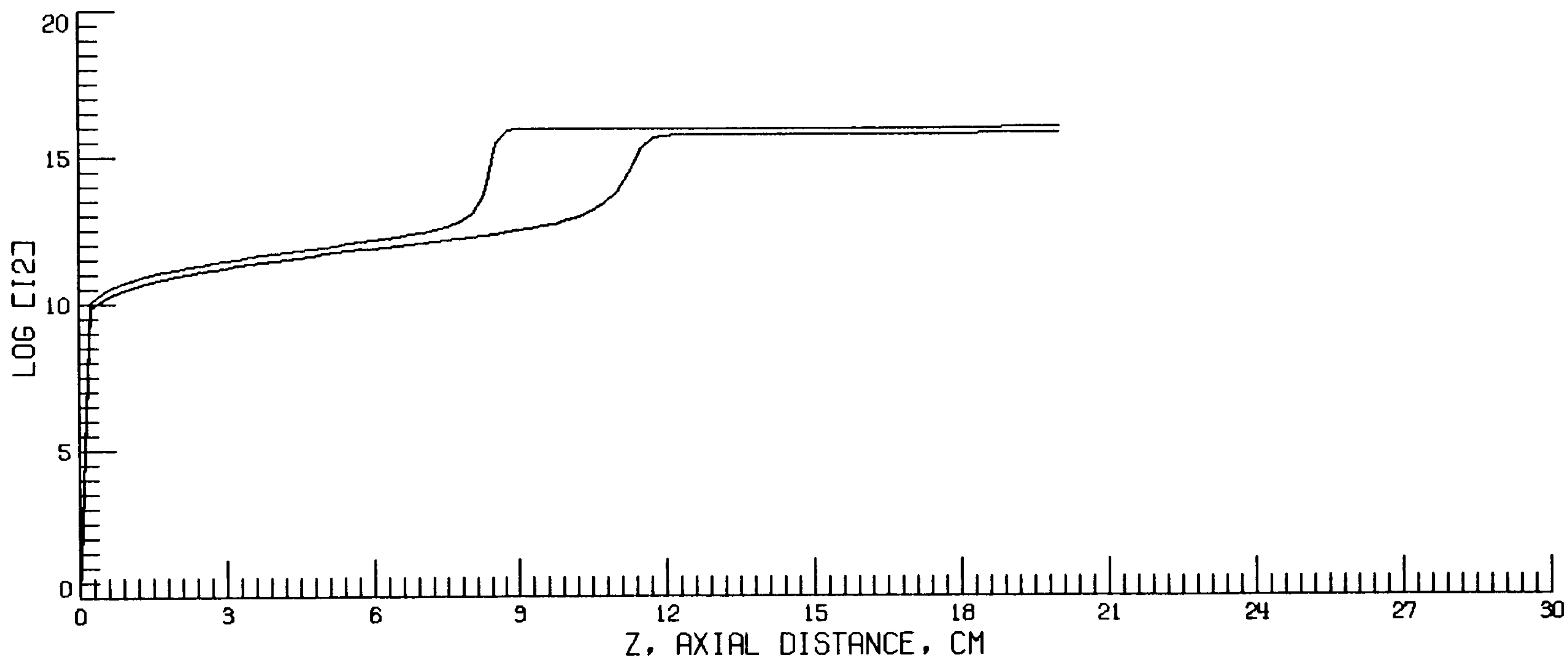

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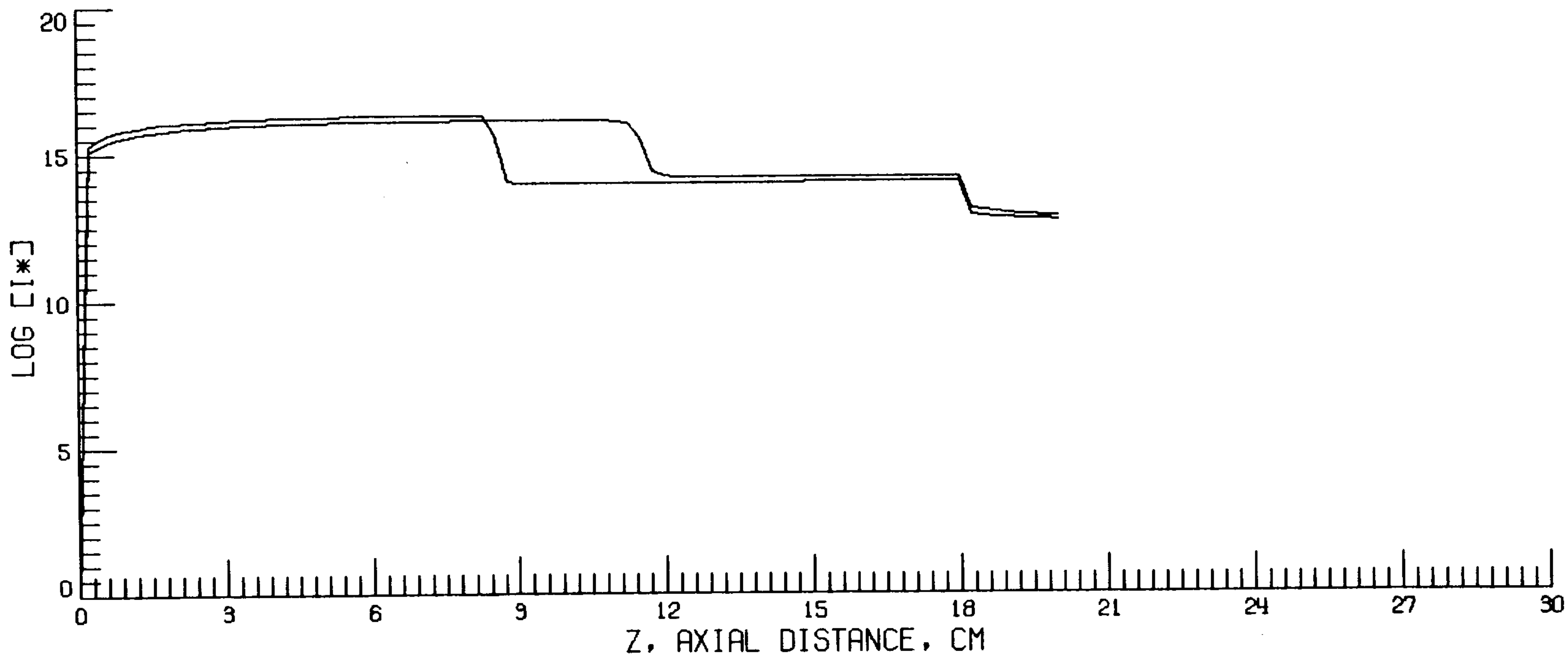

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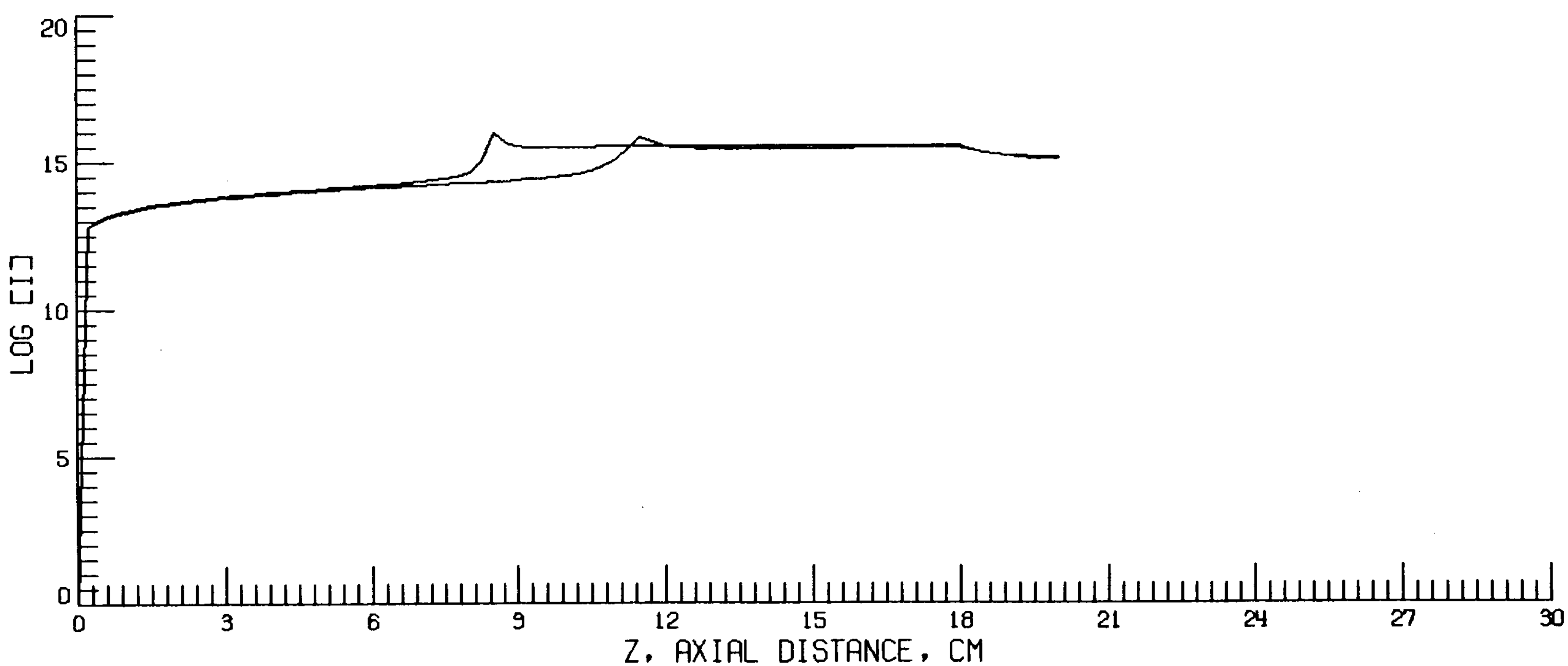

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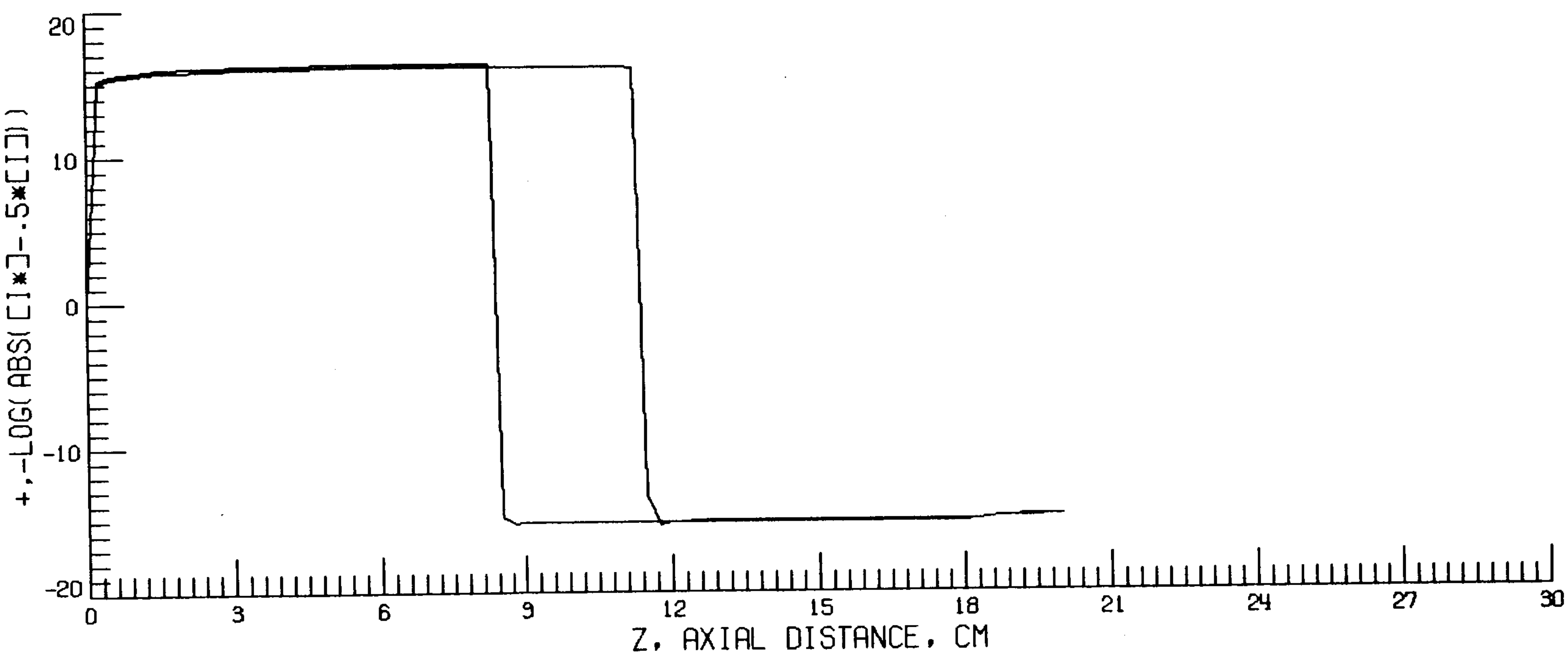

+,-LOG(ABS([I*]-.5*[I]))
20
10
0
-10
-20
0
3
6
9
12
15
18
21
24
27
30
Z, AXIAL DISTANCE, CM

INFOPLT 5.